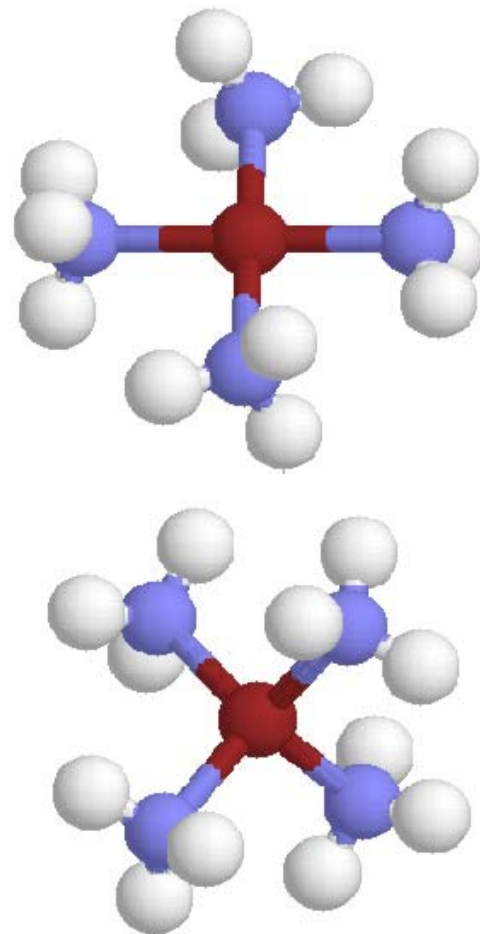


Energetics of Transition Metal Ions in Biomolecules

Anders Carlsson, Washington University, St. Louis, DMR-9971476

Transition metals interacting with biomolecules can have a profound impact on their structure and function - they can be the active site for the function of the biomolecule, act like glue to stabilize its structure, or switch its function on and off. With the increasing importance of biosensor technology and growing impact of physics in biology, understanding the interactions of transition metals with biomolecules becomes a high priority. We have studied these interactions by using highly precise energy calculations of small model molecules which mimic the transition metal environment in a biomolecule. In the model molecules shown here, a central transition metal is surrounded by four ammonia molecules. We compare the energies of different packings of the ligands to understand the structural preferences.



Energetics of Transition Metals in Biomolecules

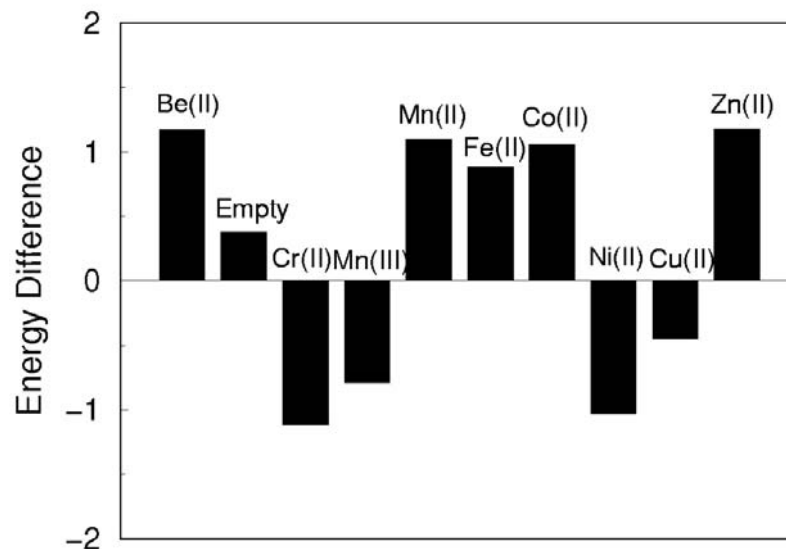
Anders Carlsson, Washington University, St. Louis, DMR-9971476

These are some of our results for different ions, showing how the interactions differ from ion to ion. This could be used in applications such as selective sensors.

Brief summary of outreach activities:

The PI has participated actively in the University City Science Advisory Council, an organization that works to improve science teaching in the University City School District, which serves a high proportion of disadvantaged students.

Graduate students who have worked on this project: Silvina Zapata, Richard Hennig, and Xueping Yu



The energy difference that we calculate is that between square and tetrahedral packings of the same transition metal